

# Special Topics on Basic EECS I

## VLSI Devices

### Lecture 2

Sung-Min Hong ([smhong@gist.ac.kr](mailto:smhong@gist.ac.kr))

Semiconductor Device Simulation Laboratory  
School of Electrical Engineering and Computer Science  
Gwangju Institute of Science and Technology

# 1D space with a flat potential (Free electron)

- Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) = E\psi(x)$$

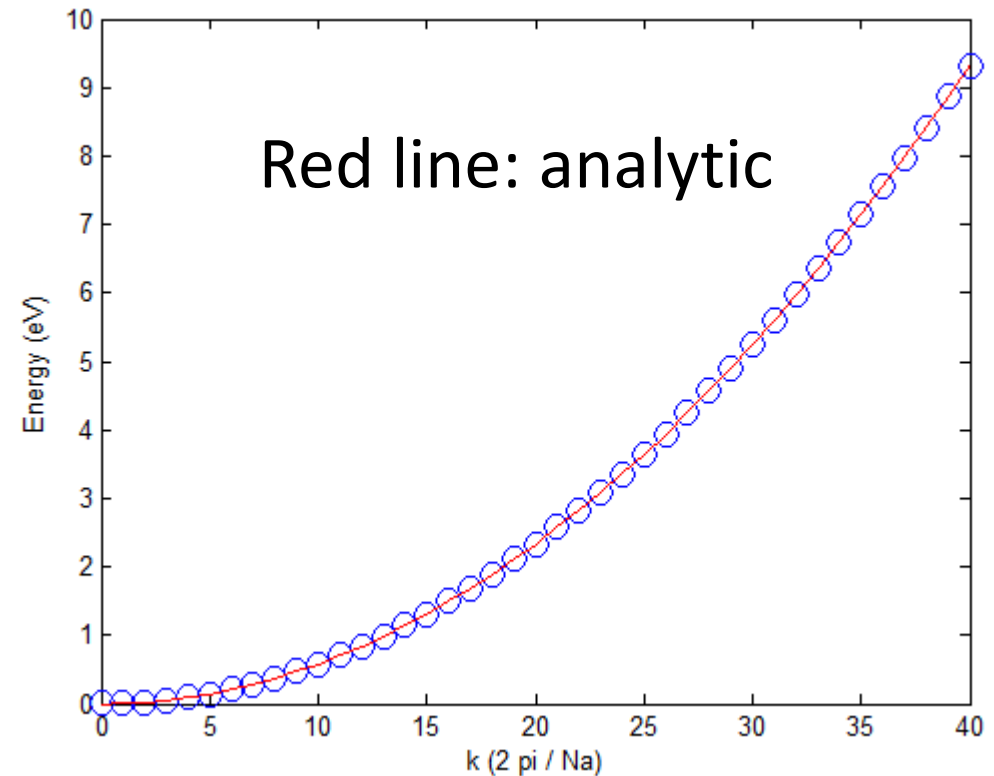
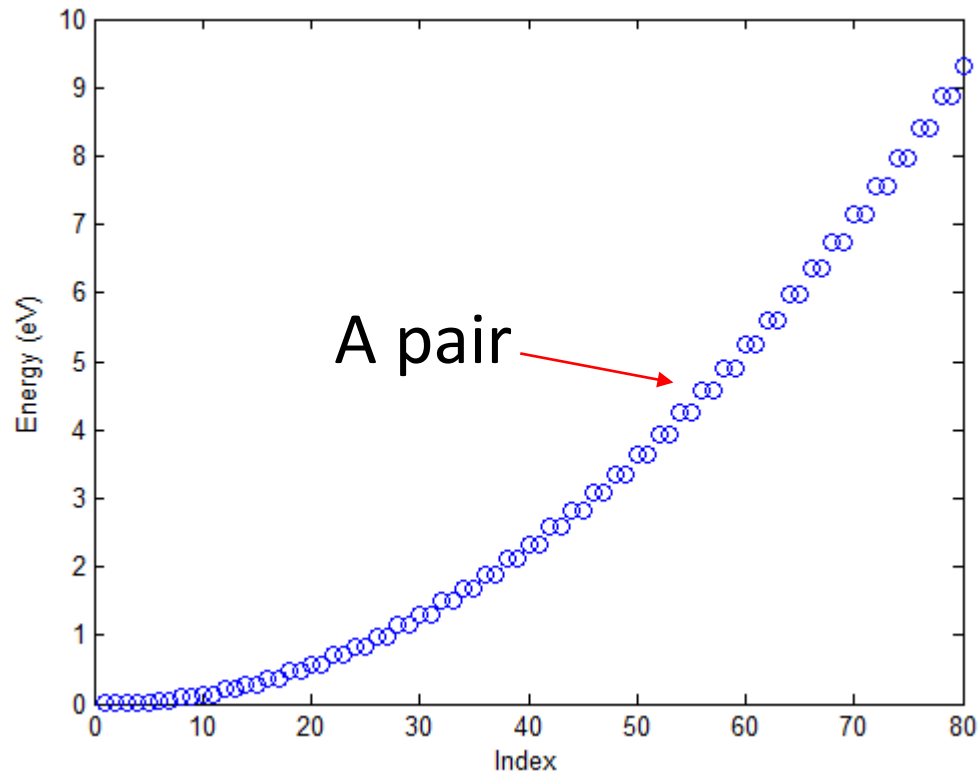
- Periodic boundary condition,  $\psi(0) = \psi(Na)$ .
- Its solution

$$\psi(x) \propto \exp\left(i \frac{2\pi}{Na} nx\right) = \exp i k x \quad \leftarrow \text{Plane wave}$$
$$E = \frac{\hbar^2}{2m} k^2$$

- $k$  can be used to identify a state.

# Numerical example (Free electron)

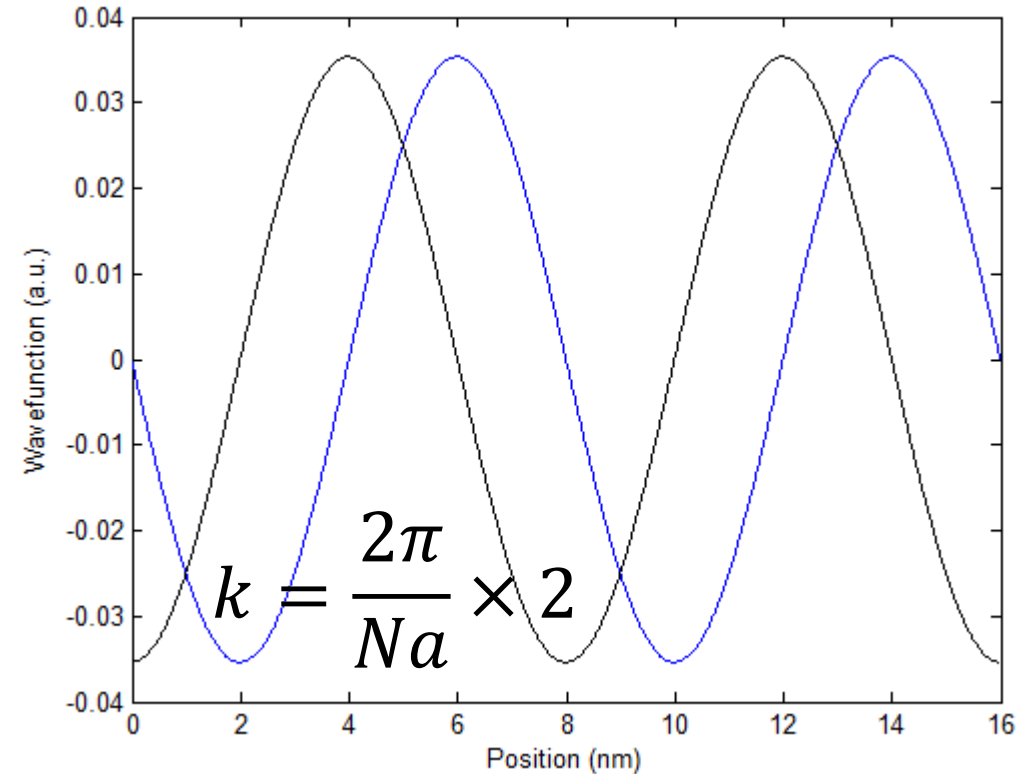
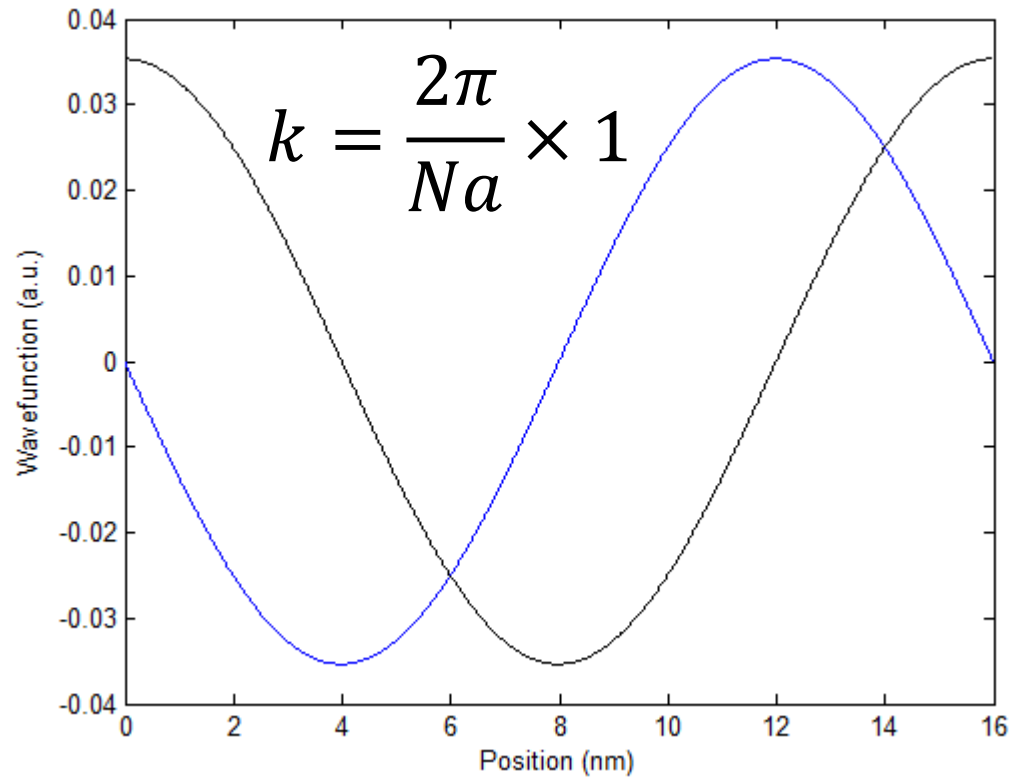
- When  $a$  is 0.4 nm and  $N$  is 40,  
– 80 states with lowest energies



# Pair?

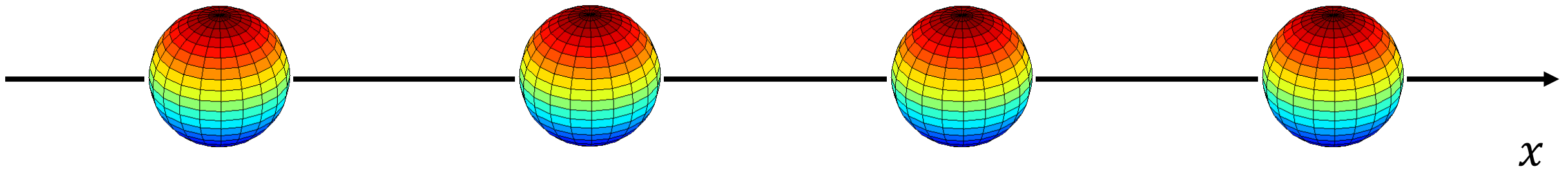
- Two sinusoidal wavefunctions with the same period

$$\exp ikx = \cos kx + i \sin kx, \exp(-ikx) = \cos kx - i \sin kx$$



# Periodicity

- Atoms are placed in a periodic manner.
  - They are attracting electrons. (Negative potential)

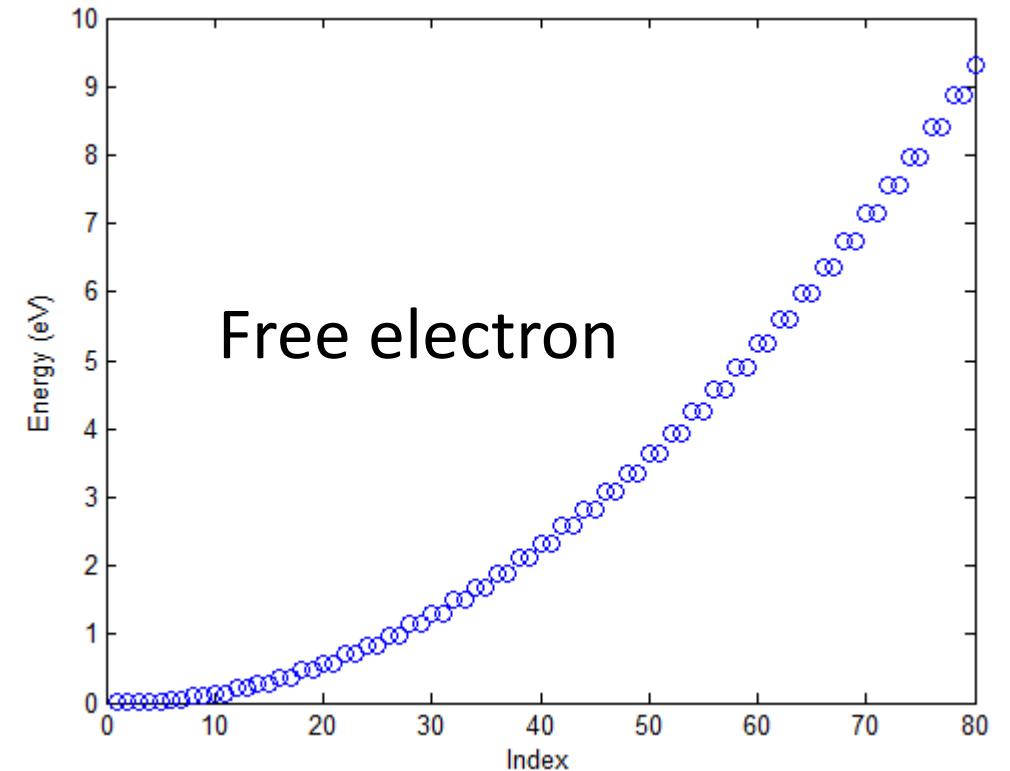
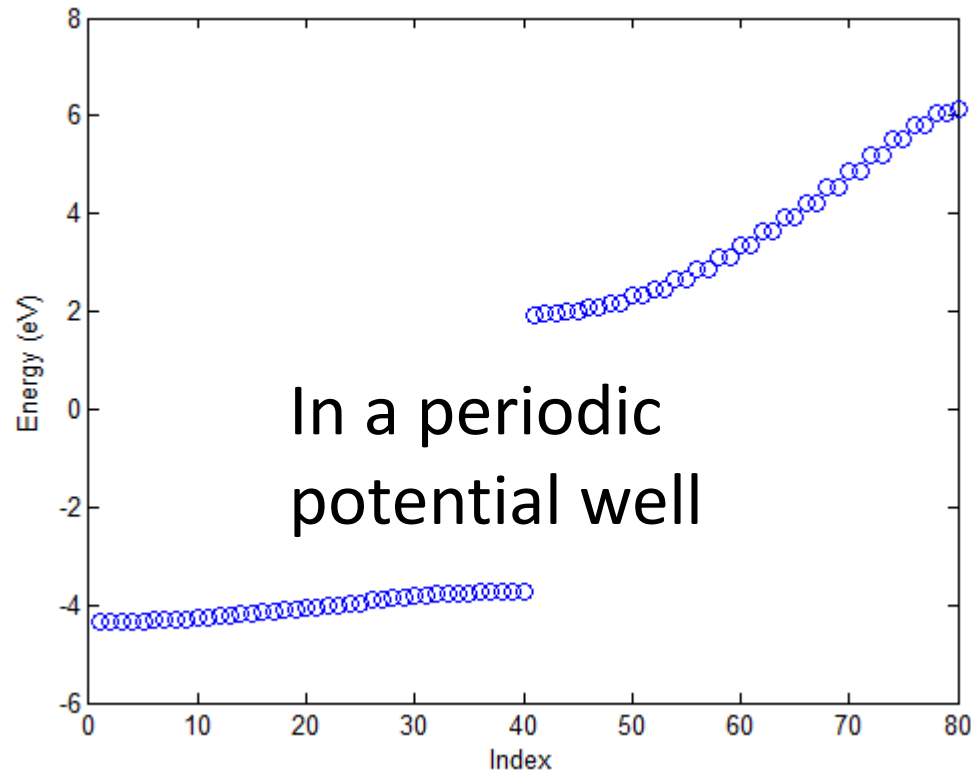


- Let us consider a periodic potential well.



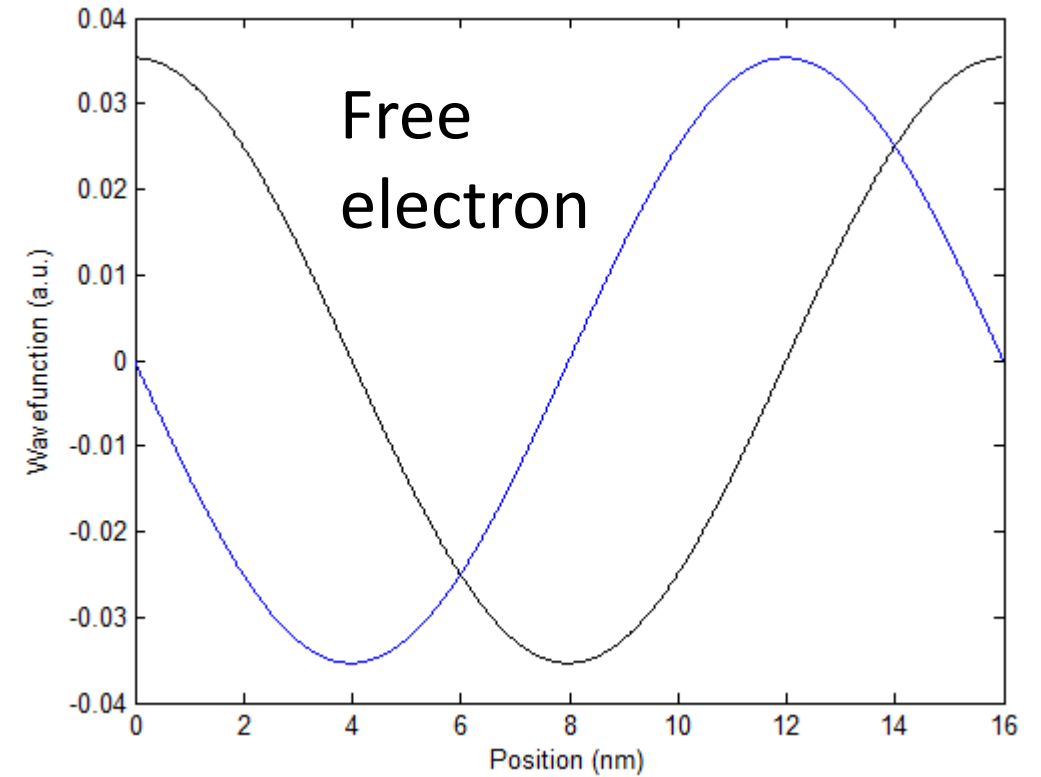
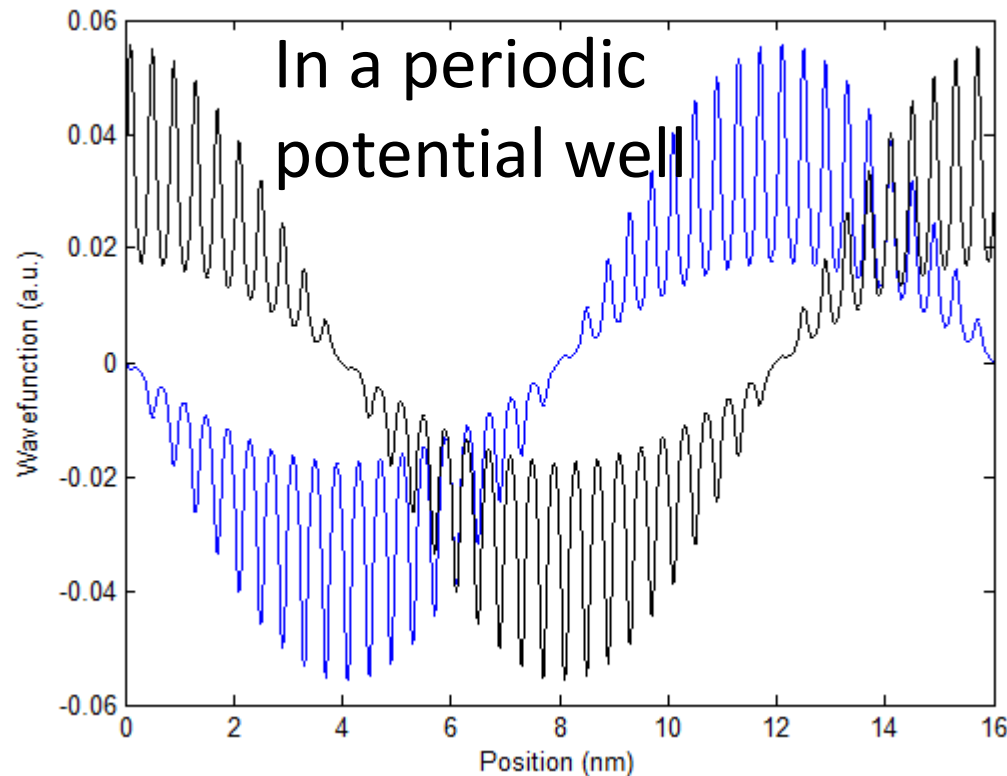
# Numerical example (Periodic potential well)

- When  $a$  is 0.4 nm,  $N$  is 40, the well width is 10 nm, and the well depth is 10.0 eV,



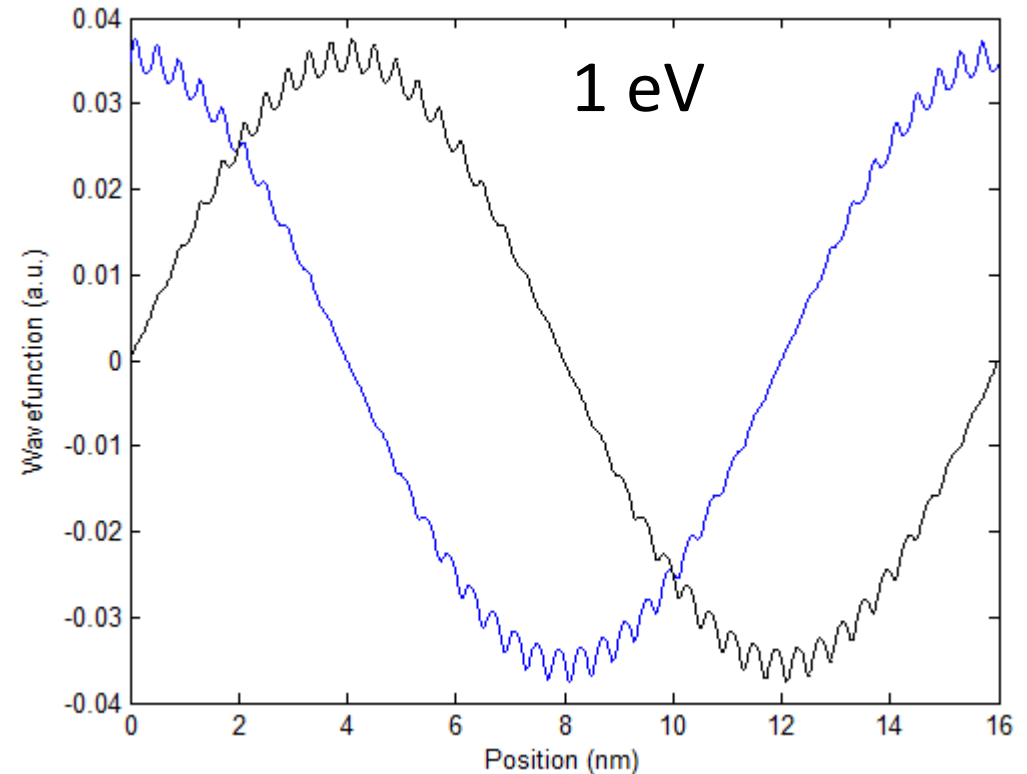
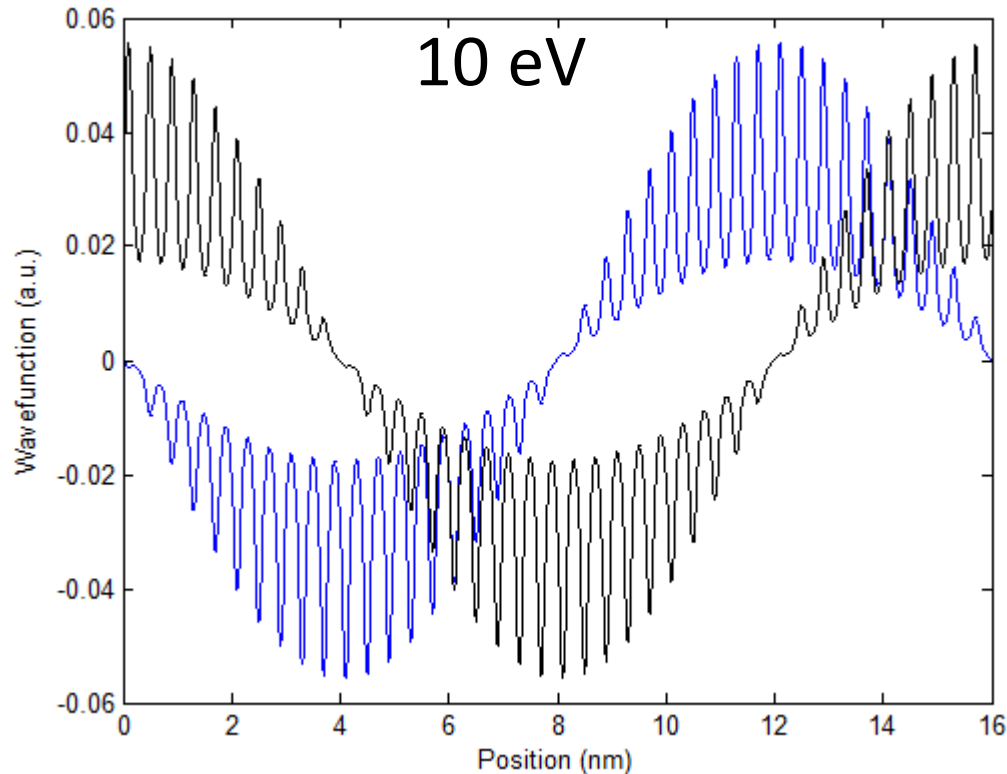
# Wavefunction (Periodic potential well)

- When  $a$  is 0.4 nm,  $N$  is 40, the well width is 0.1 nm, and the well depth is 10.0 eV,



# Observation

- $\psi(x)$  in a periodic potential well is a modulated version of the free electron wave function.





# Bloch theorem

- Under a periodic potential, the wavefunction can be expressed in a form of

$$\psi(\mathbf{r}) = u(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$$

–  $u(\mathbf{r})$  is periodic within the direct lattice.

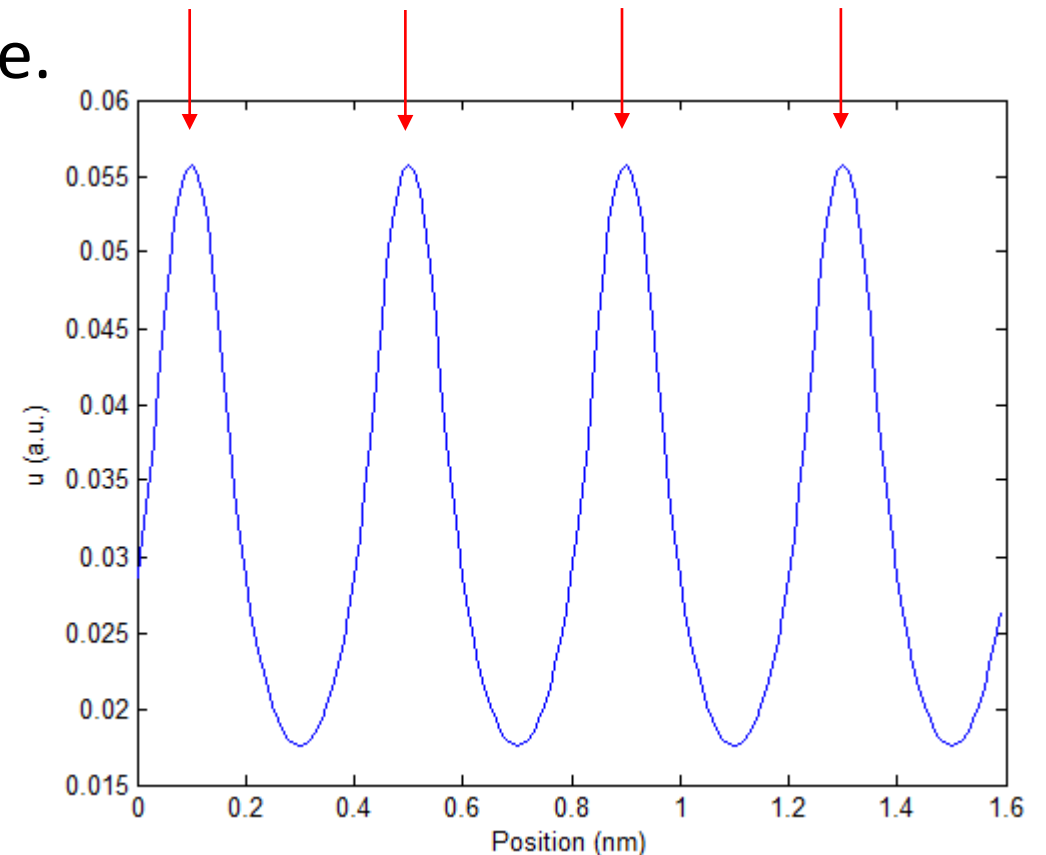
$$u(\mathbf{r} + \mathbf{R}) = u(\mathbf{r})$$

$$\mathbf{R} = i\mathbf{a}_1 + j\mathbf{a}_2 + k\mathbf{a}_3$$

–  $\mathbf{k}$  can be used to identify a state, still.

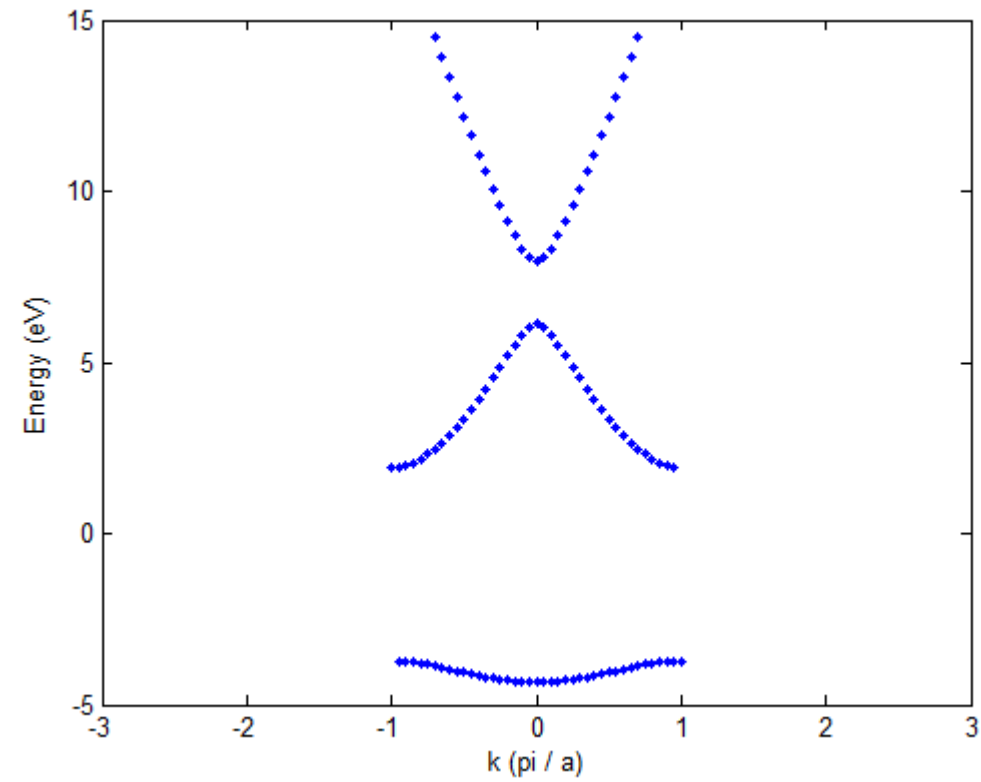
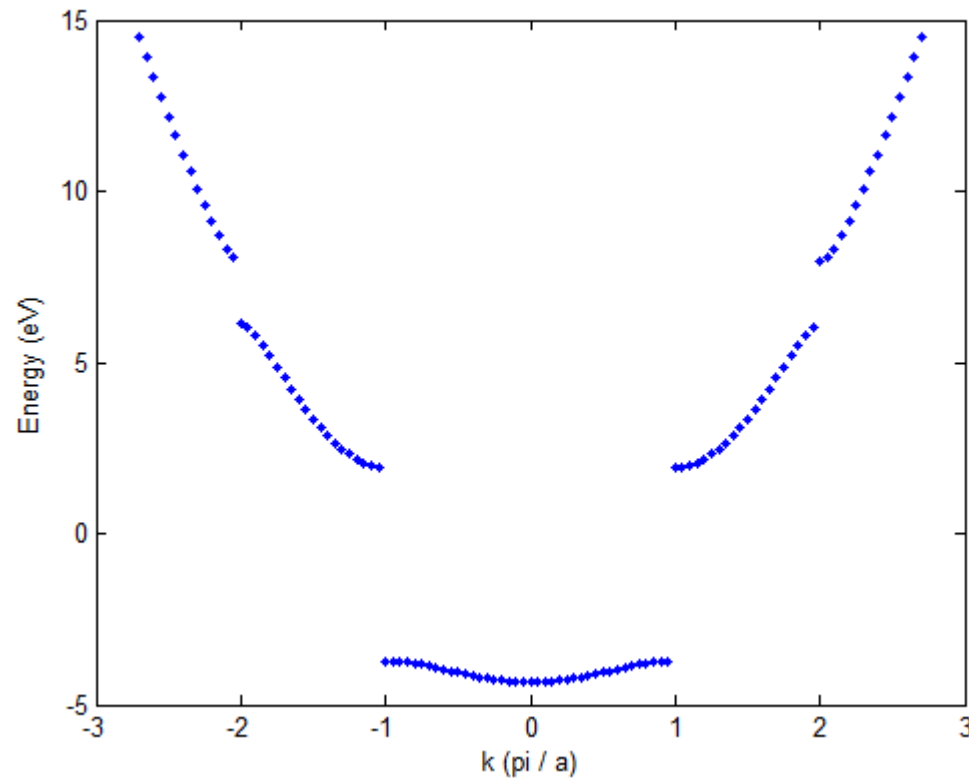
$$10 \text{ eV}, k = \frac{2\pi}{Na} \times 1$$

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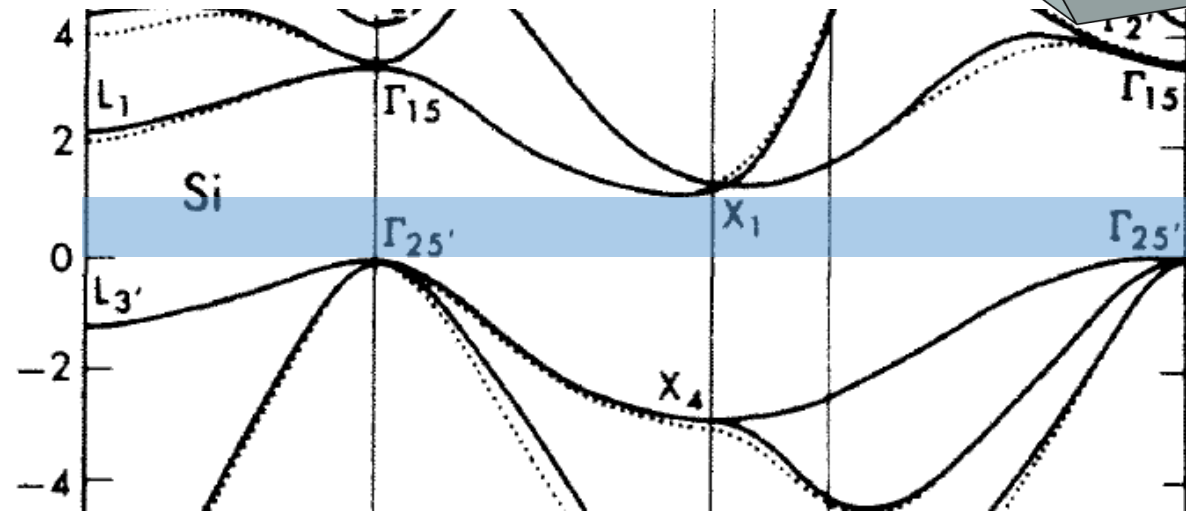
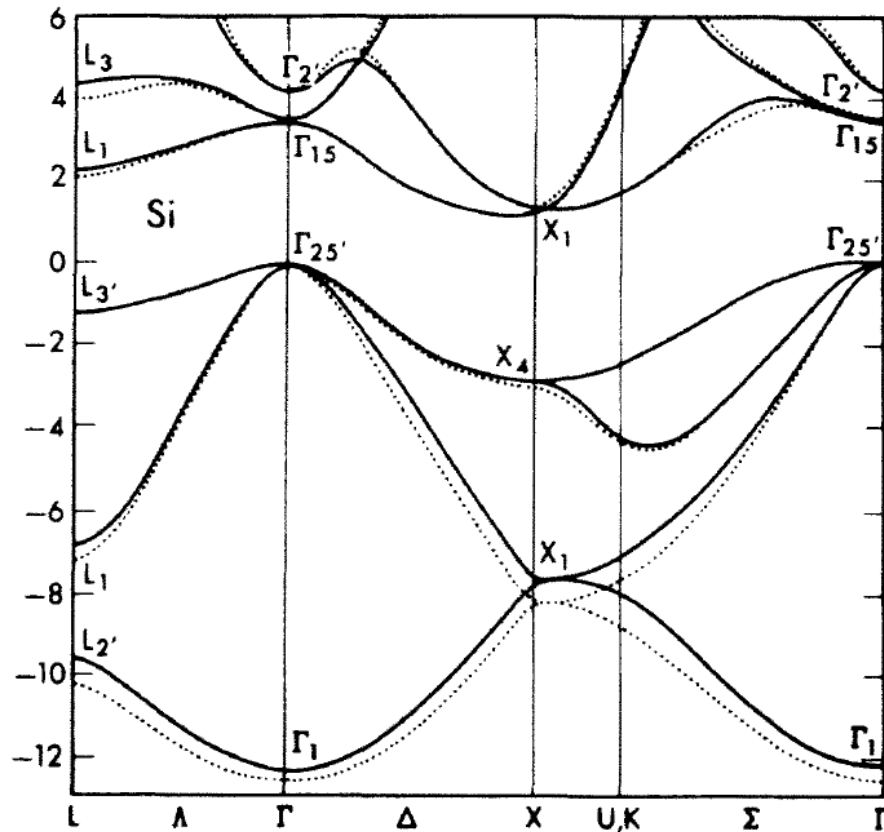
# Reduced zone scheme

- When  $\mathbf{k}$  is outside the first BZ, it is mapped onto the first BZ.

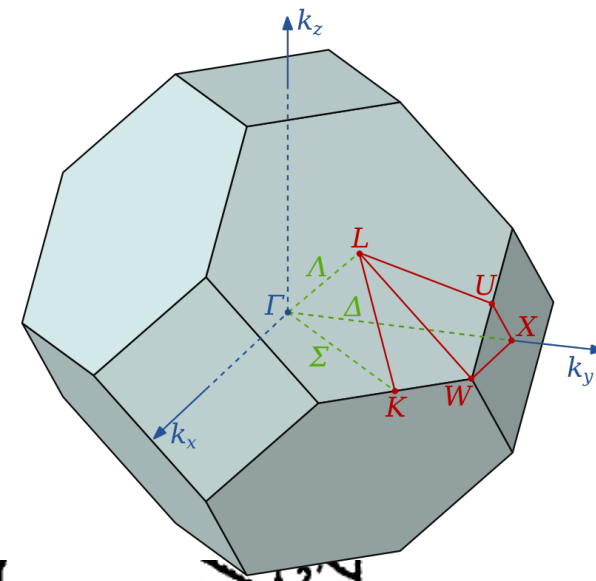


# Band structure

- We can draw the  $E - k$  diagram.
  - Bandgap is found.



Silicon band structure  
(Chelikowsky and Cohen, PRB, vol. 14,  
p. 556, 1976)



# Velocity and inverse mass

- Velocity

$$\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar} \nabla_{\mathbf{k}} E(\mathbf{k})$$

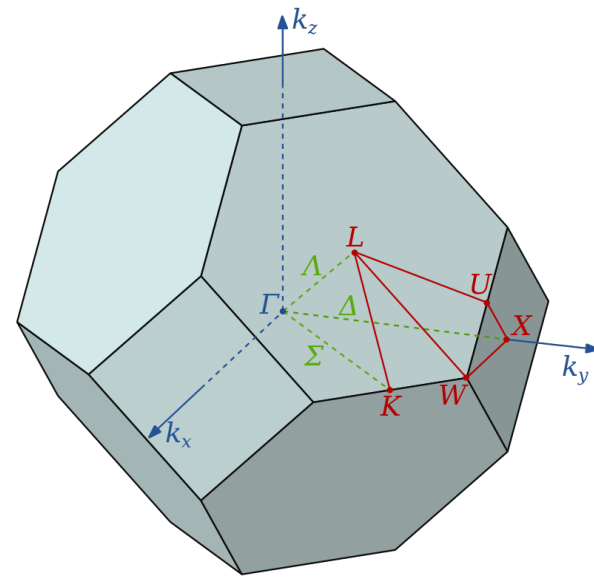
- Inverse mass (its  $ij$  component)

$$m_{ij}^{-1} = \frac{1}{\hbar} \frac{\partial}{\partial k_i} \frac{\partial}{\partial k_j} E(\mathbf{k})$$

- Example) Silicon conduction band

$$E(\mathbf{k}) - E_c = \frac{\hbar^2}{2} \left( \frac{1}{m_{xx}} k_x^2 + \frac{1}{m_{yy}} k_y^2 + \frac{1}{m_{zz}} k_z^2 \right) \quad \sim \text{Taur, Eq. (2.2)}$$

– Among three masses, one is  $m_l$  and the other two are  $m_t$ .



# Thank you!